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Technical Report

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This is the final technical report to AFOSR, which summarizes all the research activities during the period covered by the AFOSR grant. Many of the work are carried out in collaboration with S. E. Bechtel and M. G. Forest of Ohio State University. We divide these research activities into three areas, viscoelastic flows, polymeric liquid crystal flows, and Newtonian flows.

A. Viscoelastic Flows

The central theme in the study for viscoelastic flows is the modeling of thin filament flows. In particular, we want to address the issues that industries are interested in such as derivation and evaluation of reliable low-dimensional models, temperature distribution along the spinline and radial variation in fiber spinning processes and modeling of crystallization in fiber spinning processes. Our platform in addressing these issues is based on the Maxwell, Johnson-Segalman constitutive equations for the extra stress and their modifications for nonisothermal flows. Specifically, we developed a systematic way to derive and evaluate 1-D models of Maxwell and Johnson-Segalman flows, derived hybrid 2-D nonisothermal models for temperature dependent spinning processes, and studied linear and nonlinear stabilities of the flows in different geometries. The brief discuss on each of the problems is given in the following.

1. Dynamics of slender viscoelastic jets

We conducted a complete study on the 1-D model of Maxwell flows with all physical effects incorporated, such as surface tension, gravity, inertia, viscosity, and elastic relaxation. We found that the model might experience a hyperbolic to elliptic change-of-type. This catastrophic change-of-type leads to an ill-posed initial value problem for the governing 1-D model. This phenomenon does not occur if a fiber spinning process is operated at normal stable conditions. However, if the spinning is operated near an unstable state, small spatial perturbations may cause unstable temporary modes to grow persistently leading to the change-of-type. Beyond the moment of change-of-type, disturbances grow exponentially and cause filament breaks up in short time.

2. Onset of failure of stretching viscoelastic filaments

We applied a 1-D model derived from the Maxwell constitutive law to model the filament breakup phenomena in an idealized experimental setting. In this simulation, the filament is assumed hung to the “ceiling” with an uniform profile initially. Under the gravity force, it falls and drags a thin filament behind it. Our numerical simulations reveals that the model loses validity through a hyperbolic to elliptic change-of-type before the filament breaks up. Again, it is the change-of-type that foresees the arrival of small scale growth and eventual filament breakup.

3. Nonisothermal viscoelastic filament flows

The 1-D theory for thin liquid jet gives a good approximation to the essentially 3-D free boundary value problem in the isothermal modeling. In reality, however temperature distribution in the flow radial direction is not uniform and heat convects and diffuses in this direction. Therefore, the modeling must take into account the fact that the temperature distribution is really a multidimensional effect within the filament flow. In this study, we derived model energy equations by carefully selecting the time and length scales involved in the heat transport process. Based on these model equations, we studied the nonisothermal Maxwell flow under spinning conditions. The steady solutions with phase transition are computed using a premapping technique and this technique was further extended to time-dependent computations. In the time-dependent case, we developed a 2-D code to study the transient disturbance propagation and the perturbation of the phase transition in non-isothermal spinning processes. Using this hybrid 1-D and 2-D model, we were able to resolve the radial temperature distribution reasonably well and improve the prediction for the phase transition location.

4. Numerical study of interfacial instabilities in core-annular Johnson-Segalman viscoelastic flows.

In this study, we showed the existence of the radially dependent steady state in a core-annular Johnson-Segalman flow driven by a constant pressure gradient and gravity with density, Newtonian viscosity, polymer viscosity, and elastic relaxation time stratification across the fluid interface. Linearized stability of the steady state is studied for the upper-convected constitutive model. In addition to the three well-known sources of instabilities in the flow, density and viscosity stratification and surface tension, we also identified another source which is related to the jump of the first normal stress difference and shown to be proportional to the jump in the difference of relaxation and retardation times as density and total viscosity match across the interface. Numerical studies on the newly found instability with respect to various stratifications of density and total viscosity was also performed and qualitative behavior identified.

B. Study on thin liquid filaments of Polymeric liquid crystals.

Understanding the internal molecular orientation of polymeric liquids, in particular, their crystalline state near phase transition in fiber processing is of great interests and importance to the fiber manufacturing industry. We extended our perturbation technique developed for viscoelastic flows to model liquid crystal polymers using two widely accepted theories.

One is the new theory on liquid crystals with variable degree of orientation developed by Ericksen, which is developed for liquid crystals with light molecular weight. The other is the BMAB kinetic and approximate theory, a Doi type theory developed by Bhawe et al., which is suitable to liquid crystals of heavy molecular weight. We were able to conduct a thorough analysis on a wide spectrum of models derived from the theories. We summarize our work in this direction briefly in the following.

1. **Linear stability and flow-orientational interaction**

Using the approximate BMAB theory, where the kinetic BMAB theory is approximated by the Doi closure approximation, we derived self-consistent 1-D asymptotic models. We then explored the flow-orientation interaction in the model equations and found that orientation effects can suppress the hydrodynamic instability while they are dominant physical effects. In particular, the well-known Rayleigh instability for liquid crystal filaments is suppressed while the orientation energy dominates the kinetic energy.

2. **Steady state orientation prediction and their robustness**

Applying the 1-D models to fiber spinning processes, we were able to predict the orientational structure tensor not only along the centerline of the filament, but also away from the centerline for small radial variable r . At the presence of strong flows, the orientational structure tensor is essentially determined by the shape of the filament at the takeup location. The stability of the steady state are sensitive to the upstream orientation. The more oriented upstream, the less stable is the steady state in general.

3. **Asymptotic 1-D models for kinetic equations**

Using an expansion of spherical harmonics for the orientational distribution function f in the BMAB kinetic theory, we reduced the kinetic equation into an infinite dimensional dynamical system. We proposed an ansatz consistent with axisymmetric flows for the orientational structure tensor Q and systematically derived the 1-D models for thin filaments of liquid crystal polymer flows using the BMAB kinetic theory. The orientational structure tensor Q is completely determined by the first a few coefficients in the expansion of spherical harmonics. The solution of the asymptotic equations in the infinite dynamical system was then used as the "exact solution" to evaluate the 1-D models derived from approximate theories.

4. **Comparison of different closure approximations in liquid crystal theories**

In the derivation of 1-D models using BMAB theories, closure techniques are employed. So far, we have used Doi, first Hinch-Leal, and second Hinch-Leal approximation. A detailed study on steady states of thin filament flows and their linearized stabilities under fiber spinning conditions as well as nonlinear stabilities with imposed boundary perturbations had been carried out. In particular, we compared the steady solutions with respect to different closure approximations and identified the qualitative differences arisen in different approximations. We found that the hybrid Doi and the second Hinch-Leal approximation gives the most reliable solution; whereas the Doi approximation tends to overshoot for order parameters.

Moreover, we also carried out a detailed comparison between the Ericksen and BMAB theory for elongational and thin filament free surface flows and derived certain conditions for

the Ericksen theory to be applicable to liquid crystal polymers. Moreover, we demonstrated that the thin filament theory can be used to predict the free energy for the Ericksen theory through comparison with the Doi type kinetic theory.

C. Newtonian Flows

1. Study of nonlinear stabilities in the Newtonian liquid jet breakup problem using higher order perturbation schemes.

We have been studying fine local structures on the filament breakup of Newtonian liquids using a systematic perturbation scheme together with similarity solutions of the leading order equations in the perturbation scheme. We are currently working on a transient equation, whose steady state gives the similarity solution, to investigate the linear and nonlinear stability with respect to the similarity solution and anticipating that this will explain the experimentally observed cascade structure near the breakup location along the liquid filament. Moreover, we are also numerically integrating a synthetic equation consisting of higher order equations in the perturbation to create breakup conditions under periodic boundary conditions in order to evaluate the fine local structure and the weak regularization effect of surface tension in the model, furthermore, to benchmark the validity of the synthetic equation.

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